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Supporting information

Sunlight-promoted aerobic selective cyclization of olefinic amides and diselenides Jiawei Hua,^[a] Zheng Fang,^[a] Mixue Bian,^[a] Tao Ma,^[a] Man Yang,^[a] ChengKou Liu,^[a] Wei He,^[a] Zhao Yang,^[b] Kai Guo*^{[a][c]}

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1. General information

Unless otherwise indicated, all the regents and solvents were purchased from commercial suppliers and used without any further purification. ¹H spectra were recorded in CDCl₃ on 400MHz NMR spectrometers and resonances (•) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q =quartet, p = penta, dd = doublet of doublets, dt = doublet of triplets, ddt = doublet of doublet of triplets, dtd = doublet of triplet of doublets, m = multiplet, br = broad), coupling constant (J) in Hertz (Hz), and integration. ¹³C NMR were recorded at 100 MHz and chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent. Column chromatography was generally performed on Silicycle silica gel (200-300 mesh). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm coated silica gel plates (HSGF 254) and visualized the course of the reactions using a UV light (254 nm or 365 nm). High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrosprayionization-time of flight).

2. Reaction device



Figure SO. Reaction device

3. Screening of reaction conditions for O-cyclization reaction

e servering of reaction conditions for the synthesis of product ou					
N ^{-Ts} +	PhSeSePh Sunlight TFA Photocatalyst CH ₃ CN, rt	PhSe 20			
ia	2a				
Entry	Photocatalyst	Yield ^b (%)			
1	-	80			
2	Na ₂ -Eosin Y	74			
3	Eosin Y	70			
4	Acid Red 94	66			
5	Fluorescein	61			
6	-	52 ^c			
7	-	73 ^d			
8	-	7 6 ^e			

Table S0. Screening of reaction conditions for the synthesis of product 3a^a

^aReaction conditions: **1a** (0.3 mmol), **2a** (0.3 mmol), Photocatalyst (2 mol%), TFA (0.2 equiv., 0.06 mmol), CH₃CN (2.5 mL), sunlight, room temperature, air, 3h. ^bIsolated yields. ^c0.5 equiv. of **2a**. ^d0.75 equiv. of **2a**. ^e1.5 equiv. of **2a**.

4. Screening of reaction conditions for the synthesis of product 4a^a

	N ^{Ts} H + PhSeSePh	Sunlight Na ₂ -Eosin Y Na ₂ CO ₃ solvent, rt PhSe 4a	-Ts
Entry	Photocatalyst (equiv.)	Solvent	Yield ^b (%)
1	Na ₂ -Eosin Y (2 mol%)	CH ₃ CN	54
2	Na ₂ -Eosin Y (1 mol%)	CH ₃ CN	36
3	Na ₂ -Eosin Y (5 mol%)	CH₃CN	47
4	Na ₂ -Eosin Y (10 mol%)	CH₃CN	40
5	Na ₂ -Eosin Y (2 mol%)	DCE	22
6	Na ₂ -Eosin Y (2 mol%)	DMF	28
7	Na ₂ -Eosin Y (2 mol%)	DMSO	trace
8	Na ₂ -Eosin Y (2 mol%)	1,4-Dioxane	21
9	Na ₂ -Eosin Y (2 mol%)	THF	trace
10	Na ₂ -Eosin Y (2 mol%)	CH ₃ CN	50 ^c
11	Na ₂ -Eosin Y (2 mol%)	CH ₃ CN	46 ^d
12	Na ₂ -Eosin Y (2 mol%)	CH₃CN	41 ^e
13	Na ₂ -Eosin Y (2 mol%)	CH ₃ CN	30 ^f
14	Na ₂ -Eosin Y (2 mol%)	CH ₃ CN	45 ^g
15	Na ₂ -Eosin Y (2 mol%)	CH₃CN	51 ^h

Table S1. Screening of reaction conditions for the synthesis of product 4a^a

^aReaction conditions: **1a** (0.3 mmol), **2a** (0.3 mmol), Na₂-Eosin Y (equiv.), Na₂CO₃ (1 equiv.), solvent (2.5 mL), sunlight, room temperature, air, 3h. ^bIsolated yields. ^cBlue. ^dWhite. ^eGreen. ^f0.5 equiv. of **2a**. ^g0.75 equiv. of **2a**. ^h1.5 equiv. of **2a**.



5. X-ray crystallography structure of compound 3a and 4a

Figure S1. X-ray structure of 3a



Figure S2. X-ray structure of 4a

6. General procedure for the derivatization of 3s

A 35 mL glass tube was charged with substrate **3s** (0.5 mmol), 2M HCl (2mL), CH_3CN (4 mL) and a magnetic stir bar. The reaction mixture was stirred at room

temperature for overnight. After completing reaction, it was monitored with TLC. Then the reaction mixture was washed with saturated NaCl solution and extracted with ethyl acetate. The organic layer was dried with anhydrous sodium sulfate and the solvent was removed under vacuum. The pure product **5** was obtained by flash chromatography on silica gel using petroleum ether and ethyl acetate as the eluent.

7. HRMS Spectra







Figure S3-2. HRMS Spectra for compound 6

8. Fluorescence quenching experiments

The fluorescence emission intensities were recorded on spespectrofluorimeter. The

excitation wavelength was fixed at 525 nm. In a typical experiment, the emission spectrum of a 0.1 mM solution of PC in CH_3CN was collected. Then, different amount of **1a** or **2a** was added to the measured solution and the emission spectrum of the sample was collected. Here I_0 and I represent the intensities of the emission in the absence and presence of the quencher.



Figure S4. Quenching of Na2-EosinY fluorescence emission in the presence of 1a



Figure S5. Quenching of Na₂-EosinY fluorescence emission in the presence of 2a



Figure S6. Stern-volmer plots

9. Cyclic voltammetry experiment

Cyclic voltammograms of diphenyl diselenide and Na₂-EosinY were performed in a threeelectrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a steady glassy carbon disk electrode while the counter electrode was a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. (1) Diphenyl diselenide (0.3mmol) and a solvent (MeCN, 20 mL) containing "Bu₄NBF₄ (0.3 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V, -2.5 V to 0 V. (2) Na₂-EosinY (0.006mmol) and a solvent (MeCN, 20 mL) containing "Bu₄NBF₄ (0.3 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V, -2.5 V to 0 V.





Figure S7. Cyclic voltammograms of PC and 2a

10. Analytical data of compounds 3, 4, 5



(Z)-4-methyl-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3a)**. White solid (80%, 0.110g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.88 (m, 2H), 7.81 (d, *J* = 6.7 Hz, 1H), 7.44 – 7.37 (m, 2H), 7.33 (dd, *J* = 6.2, 1.8 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.19 – 7.15 (m, 1H), 7.15 – 7.09 (m, 2H), 5.79 (dd, *J* = 6.4, 4.8 Hz, 1H), 3.31 (dd, *J* = 13.3, 4.7 Hz, 1H), 3.14 (dd, *J* = 13.3, 6.6 Hz, 1H), 2.33 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.04, 145.43, 142.46, 137.18, 133.17, 132.78, 128.79, 128.26, 128.16, 127.49, 126.91, 126.82, 124.40, 121.12, 85.07, 30.27, 20.59. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₂₀NO₃SSe 458.0324 found 458.0328.



(Z)-2-methyl-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3b)**. White solid (75%, 0.103g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.83 (d, *J* = 5.2 Hz, 1H), 7.45 – 7.40 (m, 2H), 7.37 (ddt, *J* = 7.5, 5.5, 1.5 Hz, 2H), 7.30 – 7.20 (m, 4H), 7.18 – 7.15 (m, 1H), 7.15 – 7.09 (m, 2H), 5.78 (dd, *J* = 7.0, 4.2 Hz, 1H), 3.34 (dd, *J* = 13.3, 4.2 Hz, 1H),

3.08 (dd, J = 13.3, 7.0 Hz, 1H), 2.67 (s, 3H). ¹³C NMR (101 MHz, Chloroform-d) δ 166.13 , 145.58 , 138.79 , 136.88 , 133.14 , 132.82 , 131.58 , 131.07 , 128.83 , 128.36 , 128.26 , 127.86 , 127.43 , 126.92 , 124.65 , 124.26 , 121.26 , 84.98 , 30.19 , 19.68 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₂₀NO₃SSe 458.0324 found 458.0322.



(Z)-4-(tert-butyl)-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide (3c). White solid (78%, 0.117g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.87 – 7.79 (m, 1H), 7.47 – 7.37 (m, 4H), 7.35 – 7.26 (m, 3H), 7.15 (dq, *J* = 14.7, 7.2, 6.4 Hz, 3H), 5.79 (t, *J* = 5.6 Hz, 1H), 3.29 (dd, *J* = 13.3, 4.5 Hz, 1H), 3.13 (dd, *J* = 13.3, 6.7 Hz, 1H), 1.26 (s, 9H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.01, 155.39, 145.47, 137.16, 133.13, 132.83, 128.78, 128.34, 128.27, 127.53, 126.92, 126.64, 124.55, 124.45, 121.12, 85.04, 34.11, 30.25, 30.11. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₅H₂₆NO₃SSE 500.0793 found 500.0797.



(Z)-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide (**3d**). White solid (77%, 0.102g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.06 – 8.00 (m, 2H), 7.83 (d, *J* = 7.1 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.46 – 7.38 (m, 4H), 7.34 (dd, *J* = 5.8, 2.3 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.20 – 7.10 (m, 3H), 5.79 (dd, *J* = 6.5, 4.8 Hz, 1H), 3.30 (dd, *J* = 13.3, 4.6 Hz, 1H), 3.12 (dd, *J* = 13.3, 6.7 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.28 , 146.59 , 141.30 , 134.31 , 133.84 , 132.70 , 129.88 , 129.33 , 129.28 , 128.61 , 128.54 , 127.98 , 127.76 , 125.52 , 122.21 , 86.25 , 31.25 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₈NO₃SSe 444.0167 found 444.0162.



(Z)-4-methoxy-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide (3e). White solid (75%, 0.106g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 8.01 (m, 2H), 7.90 – 7.82 (m, 1H), 7.48 – 7.42 (m, 2H), 7.38 – 7.28 (m, 3H), 7.25 – 7.13 (m, 3H), 6.99 – 6.93 (m, 2H), 5.89 (t, J = 5.3 Hz, 1H), 3.82 (s, 3H), 3.35 (dd, J = 13.4, 4.8 Hz, 1H), 3.27 (dd, J = 13.4, 6.0 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-d) δ 166.96 , 163.04 , 146.41 , 134.27 , 133.68 , 132.87 , 130.04 , 129.83 , 129.25 , 128.73 , 127.83 , 125.23 , 122.20 , 113.80 , 86.23 , 55.69 , 31.48 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₂₀NO₄SSe 474.0273 found 474.0279.



(Z)-4-fluoro-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3f)**. White solid (79%, 0.109g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.02 (ddd, *J* = 10.0, 5.1, 2.5 Hz, 2H), 7.81 – 7.71 (m, 1H), 7.42 – 7.35 (m, 2H), 7.30 – 7.25 (m, 1H), 7.24 – 7.19 (m, 2H), 7.16 – 7.03 (m, 5H), 5.82 (t, *J* = 5.4 Hz, 1H), 3.28 (dd, *J* = 13.4, 4.7 Hz, 1H), 3.18 (dd, *J* = 13.5, 6.1 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.49, 164.11 (d, *J* = 252 Hz), 145.51, 136.27 (d, *J* = 3 Hz), 133.44, 132.70, 129.56 (d, *J* = 9 Hz), 128.88, 128.24, 128.02, 127.51, 126.88, 124.32, 121.17, 114.77 (d, *J* = 23 Hz), 85.43, 30.34. ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -105.29. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇FNO₃SSe 462.0073 found 462.0070.



PhSe

(Z)-2-chloro-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3g)**. White solid (73%, 0.105g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.19 (d, *J* = 7.6 Hz, 1H), 7.83 (s, 1H), 7.45 – 7.38 (m, 4H), 7.38 – 7.32 (m, 2H), 7.29 – 7.25 (m, 2H), 7.18 – 7.08 (m, 3H), 5.77 (dd, *J* = 6.6, 4.6 Hz, 1H), 3.30 (dd, *J* = 13.3, 4.5 Hz, 1H), 3.08 (dd, *J* = 13.3, 6.8 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.44 , 146.71 , 139.40 , 134.44 , 133.81 , 133.52 , 132.75 , 131.60 , 130.54 , 129.96 , 129.31 , 129.13 , 128.50 , 127.94 , 126.72 , 125.55 , 122.27 , 86.39 , 31.11 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇ClNO₃SSE 477.9777 found 477.9770.



(Z)-4-chloro-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3h)**. White solid (80%, 0.114g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.94 (m, 2H), 7.83 (d, *J* = 7.1 Hz, 1H), 7.48 – 7.38 (m, 4H), 7.38 – 7.34 (m, 1H), 7.34 – 7.28 (m, 2H), 7.20 – 7.11 (m, 3H), 5.82 (dd, *J* = 6, 5.2 Hz, 1H) , 3.33 (dd, *J* = 13.3, 4.8 Hz, 1H), 3.18 (dd, *J* = 13.3, 6.5 Hz, 1H). ¹³C NMR (101

MHz, Chloroform-*d*) δ 166.44 , 145.63 , 138.81 , 138.12 , 133.43 , 132.87 , 128.93 , 128.35 , 128.28 , 128.12 , 127.86 , 127.40 , 127.03 , 124.54 , 121.15 , 85.39 , 30.21 . HRMS (TOF) m/z [M + H]^+ Calcd for C_{21}H_{17}CINO_3SSe 477.9777 found 477.9772.



(Z)-2-bromo-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide (**3i**). White solid (74%, 0.115g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.27 – 8.19 (m, 1H), 7.86 (d, *J* = 6.8 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.42 (dq, *J* = 20.8, 6.7, 6.3 Hz, 4H), 7.31 (dd, *J* = 10.9, 7.5 Hz, 3H), 7.15 (dq, *J* = 14.3, 6.8 Hz, 3H), 5.78 (dd, *J* = 6, 4.8 Hz, 1H), 3.32 (dd, *J* = 13.3, 4.4 Hz, 1H), 3.09 (dd, *J* = 13.3, 6.9 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.32 , 145.71 , 140.17 , 134.06 , 133.37 , 132.79 , 132.41 , 129.69 , 128.93 , 128.30 , 128.16 , 127.47 , 126.92 , 126.27 , 124.57 , 121.23 , 119.87 , 85.35 , 30.07 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇BrNO₃SSE 521.9272 found 521.9278.



(Z)-3-bromo-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3j)**. White solid (73%, 0.114g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.24 (t, *J* = 1.8 Hz, 1H), 8.03 (ddd, *J* = 7.9, 1.6, 1.0 Hz, 1H), 7.86 (dd, *J* = 6.1, 2.5 Hz, 1H), 7.67 (ddd, *J* = 8.0, 1.9, 1.0 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.31 – 7.27 (m, 2H), 7.23 – 7.18 (m, 1H), 7.18 – 7.12 (m, 2H), 5.93 (t, *J* = 5.2 Hz, 1H), 3.38 (dd, *J* = 13.5, 4.6 Hz, 1H), 3.28 (dd, *J* = 13.5, 6.0 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.95, 146.64, 143.01, 135.75, 134.64, 133.67, 130.74, 130.37, 129.97, 129.27, 128.91, 128.62, 127.88, 126.42, 125.35, 122.45, 122.28, 86.64, 31.39 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇BrNO₃SSe 521.9272 found 521.9280.



(Z)-4-bromo-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3k)**. White solid (79%, 0.124g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 – 7.87 (m, 2H), 7.82 (d, *J* = 7.1 Hz, 1H), 7.60 – 7.54 (m, 2H), 7.43 (tt, *J* = 7.3, 3.8 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.34 – 7.29 (m, 2H), 7.22 – 7.11 (m, 3H), 5.81 (dd, *J* = 6.4, 4.8 Hz, 1H), 3.32 (dd, *J* = 13.3, 4.8 Hz, 1H), 3.18 (dd, *J* = 13.3, 4.8 Hz, 2H), 7.43 (tt, *J* = 7.3, 3.8 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.34 – 7.29 (m, 2H), 7.22 – 7.11 (m, 3H), 5.81 (dd, *J* = 6.4, 4.8 Hz, 1H), 3.32 (dd, *J* = 13.3, 4.8 Hz, 1H), 3.18 (dd, J = 13.8 Hz, 1H), 3.8 Hz,

6.5 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.47 , 145.63 , 139.34 , 133.45 , 132.87 , 130.85 , 128.93 , 128.39 , 128.34 , 128.10 , 127.41 , 127.02 , 126.65 , 124.53 , 121.15 , 85.41 , 30.22 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇BrNO₃SSe 521.9272 found 521.9275.



(Z)-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

(trifluoromethyl)benzenesulfonamide **(3I)**. White solid (69%, 0.106g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.2 Hz, 2H), 7.78 – 7.72 (m, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.27 – 7.21 (m, 1H), 7.19 – 7.14 (m, 2H), 7.11 – 7.06 (m, 1H), 7.05 – 6.99 (m, 2H), 5.82 (t, *J* = 5.3 Hz, 1H), 3.28 – 3.16 (m, 2H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 168.17, 146.73, 144.81, 134.70, 134.17 (t, *J* = 32.6 Hz), 133.71, 129.98, 129.27, 128.87, 128.55, 128.37, 127.90, 125.81 (q, *J* = 3.6 Hz), 125.37, 123.40 (q, *J* = 271.3 Hz), 122.26, 86.78, 31.34. ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -62.88. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₇F₃NO₃SSe 512.0041 found 512.0046.



(Z)-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

(trifluoromethoxy)benzenesulfonamide **(3m)**. White solid (72%, 0.114g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 8.8 Hz, 2H), 7.79 (d, *J* = 6.4 Hz, 1H), 7.44 – 7.35 (m, 2H), 7.32 – 7.28 (m, 1H), 7.24 (d, *J* = 7.9 Hz, 4H), 7.16 – 7.11 (m, 1H), 7.11 – 7.05 (m, 2H), 5.82 (t, *J* = 5.4 Hz, 1H), 3.28 (dd, *J* = 13.4, 4.8 Hz, 1H), 3.19 (dd, *J* = 13.4, 6.2 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.71 , 151.12 , 145.63 , 138.70 , 133.53 , 132.77 , 128.98 , 128.92 , 128.27 , 128.01 , 127.48 , 126.93 , 124.42 , 121.20 , 119.53 , 119.24 (q, *J* = 258 Hz), 85.55 , 30.27 . ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -57.59 . HRMS (TOF) m/z [M + H]⁺ Calcd for $C_{22}H_{17}F_3NO_4SSe$ 527.9990 found 527.9993.



(Z)-4-cyano-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3n)**. White solid (70%, 0.098g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.16 – 8.09 (m, 2H), 7.80 (d, *J* = 6.6 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.49 – 7.40 (m, 2H), 7.35 – 7.30 (m, 1H), 7.27 – 7.22 (m, 2H), 7.19

- 7.08 (m, 3H), 5.86 (t, *J* = 5.3 Hz, 1H), 3.31 (dd, *J* = 13.4, 4.7 Hz, 1H), 3.22 (dd, *J* = 13.5, 6.1 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.26 , 145.71 , 144.33 , 133.76 , 132.73 , 131.49 , 129.03 , 128.32 , 127.79 , 127.38 , 127.01 , 124.49 , 121.21 , 116.56 , 115.18 , 85.77 , 30.24 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₇N₂O₃SSe 469.0120 found 469.0135.



(Z)-4-nitro-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(30)**. White solid (61%, 0.089g). ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.48 – 8.42 (m, 2H), 8.33 – 8.27 (m, 2H), 7.94 (d, *J* = 7.4 Hz, 1H), 7.71 – 7.56 (m, 3H), 7.29 – 7.17 (m, 5H), 6.39 (t, *J* = 4.4 Hz, 1H), 3.70 (dd, *J* = 13.6, 4.4 Hz, 1H), 3.63 (dd, *J* = 13.6, 4.7 Hz, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 169.09, 150.28, 147.83, 146.70, 135.48, 132.44, 130.47, 129.53, 129.50, 129.47, 128.53, 127.52, 125.11, 124.82, 123.20, 88.04, 30.86. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇N₂O₅SSe 489.0018 found 489.0027.



(Z)-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)methanesulfonamide **(3p)**. White solid (77%, 0.088g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 6.1 Hz, 1H), 7.44 – 7.32 (m, 3H), 7.27 – 7.21 (m, 2H), 7.12 – 7.01 (m, 3H), 5.88 (dd, *J* = 6.2, 4.3 Hz, 1H), 3.43 (dd, *J* = 13.5, 4.3 Hz, 1H), 3.30 (dd, *J* = 13.5, 6.2 Hz, 1H), 3.04 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.28 , 146.72 , 134.49 , 133.59 , 129.92 , 129.29 , 128.88 , 128.64 , 127.81 , 125.07 , 122.34 , 86.38 , 42.20 , 31.36 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₆H₁₆NO₃SSe 382.0011 found 382.0019.



PhSe

(Z)-N-(3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)ethanesulfonamide **(3q)**. White solid (74%, 0.087g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 7.1 Hz, 1H), 7.41 (ddt, *J* = 10.9, 7.1, 3.6 Hz, 3H), 7.29 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.15 – 7.03 (m, 3H), 5.85 (dd, *J* = 6.5, 4.2 Hz, 1H), 3.47 (dd, *J* = 13.4, 4.1 Hz, 1H), 3.25 (dd, *J* = 13.4, 6.7 Hz, 1H), 3.14 (qd, *J* = 7.3, 2.0 Hz, 2H), 1.36 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.42, 146.74, 134.35, 133.67, 129.87, 129.29, 129.05, 128.60, 127.84, 125.09, 122.39, 86.10, 48.82, 31.31, 8.30. HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₇H₁₈NO₃SSE 396.0167 found 396.0159.



(Z)-4-methyl-N-(6-methyl-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-

ylidene)benzenesulfonamide **(3r)**. White solid (80%, 0.113g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.52 (s, 1H), 7.21 – 7.14 (m, 4H), 7.13 – 7.07 (m, 3H), 7.06 – 7.00 (m, 2H), 5.73 (t, *J* = 5.3 Hz, 1H), 3.23 (dd, *J* = 13.4, 4.7 Hz, 1H), 3.11 (dd, *J* = 13.4, 6.0 Hz, 1H), 2.27 (s, 3H), 2.24 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.41 , 143.99 , 143.48 , 140.17 , 138.34 , 135.48 , 133.60 , 129.34 , 129.21 , 129.15 , 128.79 , 127.84 , 127.73 , 125.11 , 121.94 , 86.21 , 31.66 , 21.61 , 21.21 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₃SSe 472.0480 found 472.0471.



(Z)-4-methyl-N-(5-methyl-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-

ylidene)benzenesulfonamide **(3s)**. White solid (78%, 0.111g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.28 – 7.21 (m, 3H), 7.21 – 7.17 (m, 2H), 7.17 – 7.08 (m, 3H), 7.04 (s, 1H), 5.75 (dd, *J* = 6, 4.8 Hz, 1H), 3.28 (dd, *J* = 13.4, 4.5 Hz, 1H), 3.14 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.33 (s, 3H), 2.24 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.20, 145.90, 144.78, 142.32, 137.45, 132.82, 129.97, 128.15, 128.11, 127.66, 126.86, 126.83, 125.78, 124.17, 121.51, 84.76, 30.41, 21.02, 20.57. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₃SSe 472.0480 found 472.0489.



(Z)-N-(6-chloro-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3t)**. White solid (82%, 0.120g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 8.3 Hz, 2H), 7.67 (s, 1H), 7.19 (d, *J* = 8.1 Hz, 3H), 7.16 – 7.08 (m, 4H), 7.03 (t, *J* = 7.3 Hz, 2H), 5.82 (dd, *J* = 5.6, 4.4 Hz, 1H), 3.30 (dd, *J* = 13.6, 4.1 Hz, 1H), 3.16 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.30 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.77, 144.63, 143.81, 137.95, 135.97, 134.18, 133.63, 131.10, 129.30, 129.20, 128.65, 127.88, 127.85, 124.78, 123.58, 86.06, 31.69, 21.65. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₉CINO₃SSe 491.9934 found 491.9942.



(Z)-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-one O-methyl oxime **(3u)**. White solid (81%, 0.080g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.55 (dd, *J* = 6.5, 1.5 Hz, 1H), 7.38 – 7.34 (m, 2H),

7.34 – 7.31 (m, 1H), 7.24 (pd, J = 7.3, 1.2 Hz, 2H), 7.13 – 7.06 (m, 3H), 5.60 (dd, J = 7.0, 4.4 Hz, 1H), 3.82 (s, 3H), 3.36 (dd, J = 13.1, 4.4 Hz, 1H), 3.13 (dd, J = 13.1, 7.1 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 155.66 , 143.28 , 133.47 , 130.65 , 129.20 , 129.15 , 129.12 , 128.86 , 127.56 , 122.19 , 121.59 , 83.91 , 62.70 , 32.19 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₆H₁₆NO₂Se 334.0341 found 334.0331.



(Z)-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-one O-isopropyl oxime **(3v)**. White solid (77%, 0.083g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.57 (dd, *J* = 6.2, 1.8 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.37 (dd, *J* = 6.0, 2.1 Hz, 1H), 7.30 – 7.21 (m, 2H), 7.11 (qd, *J* = 4.9, 1.7 Hz, 3H), 5.63 (dd, *J* = 7.4, 4.0 Hz, 1H), 4.24 (p, *J* = 6.2 Hz, 1H), 3.41 (dd, *J* = 13.1, 4.0 Hz, 1H), 3.12 (dd, *J* = 13.1, 7.5 Hz, 1H), 1.23 (d, *J* = 6.3 Hz, 6H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 142.12, 132.57, 129.29, 128.35, 128.12, 128.09, 127.96, 126.49, 121.09, 120.47, 82.59, 75.03, 31.36, 20.55. HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₈H₂₀NO₂Se 362.0654 found 362.0647.



(Z)-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-one O-(tert-butyl) oxime **(3w)**. White solid (82%, 0.093g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.68 (dd, *J* = 6.0, 2.4 Hz, 1H), 7.58 – 7.53 (m, 2H), 7.51 (dd, *J* = 5.5, 2.6 Hz, 1H), 7.41 – 7.34 (m, 2H), 7.24 (dd, *J* = 5.2, 1.9 Hz, 3H), 5.74 (dd, *J* = 7.5, 4.0 Hz, 1H), 3.54 (dd, *J* = 13.0, 4.1 Hz, 1H), 3.23 (dd, *J* = 13.0, 7.6 Hz, 1H), 1.37 (s, 9H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 154.20, 143.13, 133.67, 130.15, 129.91, 129.29, 129.17, 128.95, 127.56, 122.14, 121.58, 83.54, 78.86, 32.51, 27.45. HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₉H₂₂NO₂Se 376.0810 found 376.0801.



(Z)-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-one O-benzyl oxime **(3x)**. White solid (84%, 0.103g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.52 (dd, *J* = 5.6, 2.8 Hz, 1H), 7.40 – 7.28 (m, 5H), 7.26 – 7.13 (m, 5H), 7.07 (q, *J* = 6.2 Hz, 3H), 5.59 (dd, *J* = 7.0, 4.1 Hz, 1H), 5.03 (s, 2H), 3.36 (dd, *J* = 13.1, 4.2 Hz, 1H), 3.10 (dd, *J* = 13.1, 7.2 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 155.99 , 143.37 , 137.99 , 133.59 , 130.68 , 129.26 , 129.14 , 128.49 , 128.38 , 127.86 , 127.62 , 122.19 , 121.81 , 83.97 , 76.83 , 32.38 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₂₀NO₂Se 410.0654 found 410.0659.



(Z)-N-methyl-3-((phenylselanyl)methyl)isobenzofuran-1(3H)-imine **(3y)**. Yellow oil (31%, 0.030g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.66 (dt, *J* = 7.0, 3.7 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.32 – 7.24 (m, 3H), 7.12 (dd, *J* = 4.9, 1.9 Hz, 3H), 5.54 (t, *J* = 5.5 Hz, 1H), 3.22 (d, *J* = 5.6 Hz, 2H), 2.99 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 159.63, 145.17, 133.31, 131.10, 129.67, 129.13, 129.05, 127.39, 123.00, 121.74, 81.68, 34.33, 32.77. HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₆H₁₆NOSe 318.0392 found 318.0399.



(Z)-4-methyl-N-(3-((p-tolylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide (**3aa**). White solid (78%, 0.110g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.83 (d, *J* = 7.3 Hz, 1H), 7.47 – 7.38 (m, 3H), 7.23 (d, *J* = 8.0 Hz, 4H), 6.96 (d, *J* = 7.9 Hz, 2H), 5.76 (dd, *J* = 6.8, 4.9 Hz, 1H), 3.27 (dd, *J* = 13.2, 4.8 Hz, 1H), 3.06 (dd, *J* = 13.2, 6.9 Hz, 1H), 2.34 (s, 3H), 2.24 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.00 , 145.68 , 142.39 , 137.40 , 137.21 , 133.23 , 133.16 , 129.13 , 128.78 , 128.17 , 126.82 , 125.45 , 124.50 , 123.67 , 121.20 , 85.18 , 30.33 , 20.57 , 20.10 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₃SSe 472.0480 found 472.0469.



(Z)-4-methyl-N-(3-((o-tolylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide **(3ab)**. White solid (70%, 0.099g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.3 Hz, 2H), 7.79 (d, *J* = 7.2 Hz, 1H), 7.43 – 7.31 (m, 3H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.08 – 7.00 (m, 2H), 6.95 (td, *J* = 7.4, 2.0 Hz, 1H), 5.78 (dd, *J* = 6, 4.8 Hz, 1H), 3.25 (dd, *J* = 13.3, 4.7 Hz, 1H), 3.10 (dd, *J* = 13.3, 6.5 Hz, 1H), 2.31 (s, 3H), 2.19 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.04, 145.55, 142.45, 139.23, 137.32, 133.25, 132.45, 129.16, 128.79, 128.58, 128.16, 126.95, 126.81, 125.74, 125.37, 124.37, 121.07, 85.23, 29.19, 21.52, 20.56. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₃SSe 472.0480 found 472.0472.



(Z)-N-(3-(((4-methoxyphenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3ac)**. White solid (76%, 0.111g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.82 (d, *J* = 7.2 Hz, 1H), 7.48 – 7.32 (m, 3H), 7.22 (dd, *J* = 8.7, 2.6 Hz, 4H),

 $6.69 - 6.63 \text{ (m, 2H)}, 5.75 \text{ (dd, } J = 6.4, 5.2 \text{ Hz}, 1\text{H}), 3.70 \text{ (s, 3H)}, 3.19 \text{ (dd, } J = 13.3, 4.8 \text{ Hz}, 1\text{H}), 3.06 \text{ (dd, } J = 13.3, 6.6 \text{ Hz}, 1\text{H}), 2.34 \text{ (s, 3H)}. {}^{13}\text{C} \text{ NMR} \text{ (101 MHz, Chloroform-}d) \delta 166.09 , 158.88 , 145.65 , 142.42 , 137.31 , 135.44 , 133.18 , 128.77 , 128.33 , 128.16 , 126.82 , 124.44 , 121.14 , 117.43 , 113.96 , 85.18 , 54.33 , 30.95 , 20.59 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₄SSe 488.0429 found 488.0438.$



(Z)-N-(3-(((2-methoxyphenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3ad)**. White solid (69%, 0.101g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.77 (d, *J* = 7.4 Hz, 1H), 7.47 – 7.33 (m, 3H), 7.22 – 7.12 (m, 4H), 6.77 – 6.66 (m, 2H), 5.77 (dd, *J* = 7.1, 4.8 Hz, 1H), 3.77 (s, 3H), 3.37 (dd, *J* = 13.2, 4.7 Hz, 1H), 2.94 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.30 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.18 , 157.52 , 145.83 , 142.41 , 137.28 , 133.19 , 132.99 , 128.75 , 128.46 , 128.14 , 128.03 , 126.80 , 124.28 , 121.39 , 120.38 , 115.82 , 109.78 , 85.62 , 54.85 , 27.38 , 20.57 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₄SSe 488.0429 found 488.0427.



(Z)-N-(3-(((3-methoxyphenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3ae)**. White solid (74%, 0.108g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.89 (m, 2H), 7.81 (d, *J* = 6.6 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.35 – 7.30 (m, 1H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.05 (t, *J* = 7.9 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 6.80 – 6.76 (m, 1H), 6.73 – 6.68 (m, 1H), 5.80 (dd, *J* = 6.3, 4.8 Hz, 1H), 3.68 (s, 3H), 3.32 (dd, *J* = 13.3, 4.7 Hz, 1H), 3.14 (dd, *J* = 13.3, 6.6 Hz, 1H), 2.33 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.02 , 158.69 , 145.47 , 142.45 , 137.27 , 133.11 , 129.06 , 128.78 , 128.45 , 128.30 , 128.16 , 126.84 , 124.76 , 124.40 , 121.17 , 118.07 , 112.69 , 85.06 , 54.31 , 30.26 , 20.57 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₄SSe 488.0429 found 488.0432.



(Z)-N-(3-(((4-fluorophenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3af)**. White solid (83%, 0.119g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 7.7 Hz, 2H), 7.84 (d, *J* = 5.2 Hz, 1H), 7.42 (q, *J* = 7.9, 5.8 Hz, 2H), 7.26 (dt, *J* = 12.6, 6.5 Hz, 5H), 6.82 (t, *J* = 8.3 Hz, 2H), 5.82 (t, *J* = 5.2 Hz, 1H), 3.27 (dd, *J* = 13.4, 4.4 Hz, 1H), 3.18 (dd, *J* = 13.4, 6.1 Hz, 1H), 2.35 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.94 , 161.75 (d, *J* = 247 Hz) , 145.31 , 142.47 , 137.25 , 135.46 (d, *J* = 8 Hz) , 133.16 , 128.84 , 128.45 , 128.17 , 126.79 , 124.48 ,

122.13 (d, J = 4 Hz) , 120.92 , 115.43 (d, J = 21 Hz) , 84.89 , 31.18 , 20.59 . ^{19}F NMR (376 MHz, Chloroform-d) δ -112.95 . HRMS (TOF) m/z [M + H]+ Calcd for $C_{22}H_{19}\text{FNO}_3\text{SSe}$ 476.0229 found 476.0235.



(Z)-N-(3-(((4-chlorophenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3ag)**. White solid (80%, 0.118g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.0 Hz, 2H), 7.83 (s, 1H), 7.47 – 7.39 (m, 2H), 7.29 – 7.21 (m, 3H), 7.21 – 7.17 (m, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 5.83 (t, *J* = 5.2 Hz, 1H), 3.30 (dd, *J* = 13.5, 4.5 Hz, 1H), 3.21 (dd, *J* = 13.5, 6.0 Hz, 1H), 2.35 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.86 , 145.26 , 142.47 , 137.33 , 134.29 , 133.20 , 128.89 , 128.45 , 128.38 , 128.19 , 126.79 , 125.83 , 124.51 , 120.92 , 84.86 , 30.89 , 20.59 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₉ClNO₃SSe 491.9934 found 491.9941.



(Z)-N-(3-(((2-chlorophenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4methylbenzenesulfonamide **(3ah)**. White solid (73%, 0.107g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.3 Hz, 2H), 7.80 (d, *J* = 7.3 Hz, 1H), 7.45 – 7.35 (m, 3H), 7.26 – 7.18 (m, 4H), 7.09 (td, *J* = 7.7, 1.6 Hz, 1H), 7.01 (td, *J* = 7.6, 1.4 Hz, 1H), 5.84 (dd, *J* = 6, 5.2 Hz, 1H), 3.41 (dd, *J* = 13.4, 4.7 Hz, 1H), 3.15 (dd, *J* = 13.4, 6.5 Hz, 1H), 2.31 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.90 , 145.35 , 142.51 , 137.21 , 135.57 , 133.31 , 132.61 , 128.92 , 128.70 , 128.18 , 127.85 , 126.81 , 126.46 , 124.48 , 121.07 , 84.97 , 28.86 , 20.57 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₉CINO₃SSe 491.9934 found 491.9932.



(Z)-N-(3-(((4-bromophenyl)selanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-

methylbenzenesulfonamide **(3ai)**. White solid (81%, 0.130g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.3 Hz, 2H), 7.80 – 7.73 (m, 1H), 7.37 (dt, *J* = 7.4, 3.5 Hz, 2H), 7.25 – 7.12 (m, 5H), 7.09 – 7.04 (m, 2H), 5.84 (t, *J* = 5.0 Hz, 1H), 3.30 – 3.20 (m, 2H), 2.30 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.09, 146.28, 143.57, 138.28, 135.38, 134.33, 132.22, 129.90, 129.32, 129.25, 127.82, 127.78, 125.31, 122.16, 122.09, 86.08, 31.96, 21.64. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₉BrNO₃SSE 535.9429 found 535.9438.



(Z)-4-methyl-N-(3-(((4-nitrophenyl)selanyl)methyl)isobenzofuran-1(3H)-

ylidene)benzenesulfonamide **(3aj)**. White solid (51%, 0.077g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.93 (m, 2H), 7.89 (d, *J* = 8.3 Hz, 2H), 7.83 (d, *J* = 5.5 Hz, 1H), 7.44 (ddt, *J* = 9.0, 7.4, 1.9 Hz, 4H), 7.29 (dd, *J* = 5.7, 2.4 Hz, 1H), 7.23 (d, *J* = 8.3 Hz, 2H), 5.96 (t, *J* = 5.0 Hz, 1H), 3.47 (dd, *J* = 5.0, 1.8 Hz, 2H), 2.34 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.52, 145.92, 144.93, 142.56, 138.04, 137.30, 133.36, 131.35, 129.13, 128.49, 128.24, 126.65, 124.62, 122.93, 120.75, 84.63, 30.33, 20.58. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₁₉N₂O₅SSe 503.0174 found 503.0178.



(Z)-4-methyl-N-(3-((methylselanyl)methyl)isobenzofuran-1(3H)-ylidene)benzenesulfonamide (**3ak**). White solid (78%, 0.092g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.81 (d, *J* = 7.7 Hz, 1H), 7.58 (td, *J* = 7.6, 1.0 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 5.89 (t, *J* = 5.3 Hz, 1H), 2.95 (d, *J* = 5.4 Hz, 2H), 2.33 (s, 3H), 1.91 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 167.17, 147.02, 143.42, 138.48, 134.53, 129.87, 129.47, 129.23, 127.64, 125.47, 121.92, 87.43, 28.15, 21.59, 6.32. HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₇H₁₈NO₃SSe 396.0167 found 396.0172.



(Z)-N-(3-((ethylselanyl)methyl)isobenzofuran-1(3H)-ylidene)-4-methylbenzenesulfonamide (**3al**). White solid (75%, 0.092g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.82 (d, *J* = 7.7 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.52 – 7.42 (m, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 5.88 (t, *J* = 5.5 Hz, 1H), 3.01 (dd, *J* = 13.6, 5.0 Hz, 1H), 2.92 (dd, *J* = 13.5, 6.2 Hz, 1H), 2.52 (qd, *J* = 7.5, 2.4 Hz, 2H), 2.34 (s, 3H), 1.26 (t, *J* = 7.5 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.11, 146.12, 142.35, 137.50, 133.45, 128.83, 128.43, 128.20, 126.61, 124.50, 120.89, 86.47, 24.93, 20.56, 18.27, 14.64 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₈H₂₀NO₃SSe 410.0324 found 410.0329.



3-((phenylselanyl)methyl)-2-tosylisoindolin-1-one (**4a**). White solid (54%, 0.074g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (s, 2H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.32 (ddd, *J* = 9.1, 5.3, 2.2 Hz, 1H), 7.29

-7.26 (m, 2H), 7.23 (d, J = 8.1 Hz, 2H), 7.16 -7.08 (m, 3H), 7.07 -7.01 (m, 2H), 5.44 (dd, J = 6.1, 2.5 Hz, 1H), 3.73 (dd, J = 13.2, 2.5 Hz, 1H), 3.63 (dd, J = 13.2, 6.2 Hz, 1H), 2.33 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.43 , 144.14 , 143.16 , 134.79 , 132.49 , 132.26 , 128.89 , 128.64 , 128.27 , 128.12 , 127.92 , 127.20 , 126.29 , 123.67 , 122.22 , 59.89 , 31.84 , 20.68 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₂₀NO₃SSe 458.0324 found 458.0321.



2-((4-(tert-butyl)phenyl)sulfonyl)-3-((phenylselanyl)methyl)isoindolin-1-one (**4b**). White solid (58%, 0.087g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.93 (m, 2H), 7.70 (dd, *J* = 7.0, 1.3 Hz, 1H), 7.45 – 7.41 (m, 2H), 7.33 – 7.26 (m, 3H), 7.15 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.12 – 7.07 (m, 1H), 7.06 – 7.01 (m, 2H), 5.44 (dd, *J* = 6.2, 2.4 Hz, 1H), 3.74 (dd, *J* = 13.1, 2.5 Hz, 1H), 3.63 (dd, *J* = 13.1, 6.2 Hz, 1H), 1.22 (s, 9H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.44 , 156.93 , 143.22 , 134.73 , 132.51 , 132.23 , 128.90 , 128.30 , 128.12 , 127.93 , 127.02 , 126.28 , 125.05 , 123.63 , 122.27 , 59.94 , 34.24 , 31.85 , 29.96 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₅H₂₆NO₃SSE 500.0793 found 500.0798.



3-((phenylselanyl)methyl)-2-(o-tolylsulfonyl)isoindolin-1-one (**4c**). White solid (51%, 0.070g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.71 – 7.66 (m, 1H), 7.44 – 7.39 (m, 2H), 7.38 – 7.32 (m, 2H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.29 – 7.25 (m, 2H), 7.17 (s, 1H), 7.15 – 7.06 (m, 3H), 5.49 (dd, *J* = 6.9, 2.5 Hz, 1H), 3.88 (dd, *J* = 13.1, 2.5 Hz, 1H), 3.57 (dd, *J* = 13.1, 6.9 Hz, 1H), 2.48 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.07 , 143.23 , 136.97 , 135.96 , 132.99 , 132.57 , 132.28 , 131.50 , 130.33 , 128.58 , 128.25 , 128.14 , 128.00 , 126.35 , 125.36 , 123.81 , 122.50 , 60.30 , 32.06 , 19.44 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₂H₂₀NO₃SSe 458.0324 found 458.0327.





3-((phenylselanyl)methyl)-2-(phenylsulfonyl)isoindolin-1-one (**4d**). White solid (51%, 0.068g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 8.02 (m, 2H), 7.72 (d, *J* = 7.3 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.36 – 7.26 (m, 3H), 7.17 – 7.09 (m, 3H), 7.04 (t, *J* = 7.3 Hz, 2H), 5.46 (dd, *J* = 6.0, 2.5 Hz, 1H), 3.73 (dd, *J* = 13.2, 2.5 Hz, 1H), 3.64 (dd, *J* = 13.2, 6.1 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.41, 143.14, 137.74, 133.03, 132.57, 132.30, 128.80, 128.20, 128.17, 128.04, 127.94, 127.14, 126.34, 123.73, 122.22, 59.95, 31.84. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₈NO₃SSe 444.0167 found 444.0169.



2-((4-fluorophenyl)sulfonyl)-3-((phenylselanyl)methyl)isoindolin-1-one (**4e**). White solid (47%, 0.065g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 (ddd, *J* = 9.0, 5.0, 2.5 Hz, 2H), 7.71 (d, *J* = 7.0 Hz, 1H), 7.36 – 7.23 (m, 3H), 7.10 (dtd, *J* = 8.2, 5.8, 5.0, 2.2 Hz, 5H), 7.06 – 7.00 (m, 2H), 5.46 (dd, *J* = 5.6, 2.7 Hz, 1H), 3.70 (dd, *J* = 13.2, 2.7 Hz, 1H), 3.65 (dd, *J* = 13.2, 5.6 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.44, 164.87 (d, *J* = 255 Hz), 143.06, 133.69 (d, *J* = 3 Hz), 132.71, 132.22, 130.16 (d, *J* = 10 Hz), 128.66, 128.25, 128.16, 127.96, 126.36, 123.69, 122.19, 115.31 (d, *J* = 23 Hz), 59.96, 31.77. ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -102.52. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇FNO₃SSe 462.0073 found 462.0077.



2-((2-chlorophenyl)sulfonyl)-3-((phenylselanyl)methyl)isoindolin-1-one (**4f**). White solid (50%, 0.071g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.34 (dd, *J* = 7.5, 2.1 Hz, 1H), 7.66 (dd, *J* = 6.3, 2.2 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.41 – 7.37 (m, 1H), 7.37 – 7.30 (m, 4H), 7.17 – 7.07 (m, 3H), 5.70 (dd, *J* = 7.0, 2.4 Hz, 1H), 3.92 (dd, *J* = 13.1, 2.5 Hz, 1H), 3.61 (dd, *J* = 13.1, 7.1 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 164.92 , 143.62 , 134.95 , 133.95 , 132.97 , 132.76 , 132.31 , 130.84 , 130.56 , 128.19 , 128.15 , 128.01 , 126.35 , 126.16 , 123.80 , 122.56 , 61.05 , 32.12 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇CINO₃SSe 477.9777 found 477.9772.



2-((4-bromophenyl)sulfonyl)-3-((phenylselanyl)methyl)isoindolin-1-one (**4g**). White solid (52%, 0.081g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.87 (m, 2H), 7.73 (d, *J* = 6.8 Hz, 1H), 7.60 – 7.54 (m, 2H), 7.38 – 7.25 (m, 3H), 7.12 (dt, *J* = 7.2, 2.5 Hz, 3H), 7.08 – 7.01 (m, 2H), 5.46 (dd, *J* = 5.8, 2.4 Hz, 1H), 3.72 (dd, *J* = 13.2, 2.5 Hz, 1H), 3.64 (dd, *J* = 13.2, 5.9 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.42 , 143.09 , 136.62 , 132.77 , 132.24 , 131.32 , 128.68 , 128.60 , 128.39 , 128.30 , 128.13 , 127.99 , 126.39 , 123.78 , 122.19 , 59.96 , 31.72 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₇BrNO₃SSe 521.9272 found 521.9278.



4-((1-oxo-3-((phenylselanyl)methyl)isoindolin-2-yl)sulfonyl)benzonitrile (**4h**). White solid (45%, 0.063g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 8.4 Hz, 2H), 7.72 (t, *J* = 8.4 Hz, 3H), 7.35

 $(dt, J = 14.9, 7.2 \text{ Hz}, 2\text{H}), 7.26 (d, J = 7.3 \text{ Hz}, 1\text{H}), 7.17 - 7.01 (m, 5\text{H}), 5.51 (dd, J = 4.5, 2.6 \text{ Hz}, 1\text{H}), 3.73 - 3.62 (m, 2\text{H}). {}^{13}\text{C} \text{ NMR} (101 \text{ MHz}, \text{Chloroform-}d) \delta 165.39 , 143.01 , 141.52 , 133.04 , 132.11 , 131.75 , 128.46 , 128.30 , 128.04 , 127.83 , 126.48 , 123.88 , 122.17 , 116.59 , 116.11 , 60.06 , 31.61 . HRMS (TOF) m/z [M + H]^+ Calcd for C_{22}H_{17}N_2O_3SSe 469.0120 found 469.0111.$



2-((4-nitrophenyl)sulfonyl)-3-((phenylselanyl)methyl)isoindolin-1-one **(4i)**. White solid (34%, 0.050g). ¹H NMR (400 MHz, Chloroform-*d*) δ 8.24 (s, 4H), 7.74 (dd, J = 6.5, 1.6 Hz, 1H), 7.36 (pd, J = 7.3, 1.2 Hz, 2H), 7.29 – 7.25 (m, 1H), 7.12 (ddt, J = 7.4, 6.2, 1.7 Hz, 1H), 7.10 – 7.01 (m, 4H), 5.53 (dd, J = 5.1, 2.8 Hz, 1H), 3.74 – 3.64 (m, 2H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.39, 149.69, 143.01, 142.96, 133.11, 132.08, 128.60, 128.49, 128.26, 128.04, 127.99, 126.50, 123.91, 123.17, 122.16, 60.08, 31.61. HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₁H₁₈N₂O₅SSe 489.0018 found 489.0010.



5-methyl-3-((phenylselanyl)methyl)-2-tosylisoindolin-1-one (**4j**). White solid (55%, 0.078g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.21 (d, *J* = 8.2 Hz, 2H), 7.10 – 7.05 (m, 4H), 7.03 – 6.97 (m, 2H), 6.93 (s, 1H), 5.40 (dd, *J* = 5.4, 2.4 Hz, 1H), 3.69 (dd, *J* = 13.3, 5.5 Hz, 1H), 3.63 (dd, *J* = 13.3, 2.5 Hz, 1H), 2.31 (s, 3H), 2.11 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 165.49 , 144.02 , 143.86 , 143.29 , 134.93 , 132.38 , 129.23 , 128.61 , 128.34 , 127.73 , 127.10 , 126.41 , 126.29 , 123.37 , 122.66 , 59.86 , 32.06 , 20.93 , 20.66 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₂₃H₂₂NO₃SSE 472.0480 found 472.0485.



2-(ethylsulfonyl)-3-((phenylselanyl)methyl)isoindolin-1-one (**4k**). White solid (55%, 0.064g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.81 (dd, *J* = 5.7, 2.8 Hz, 1H), 7.44 – 7.32 (m, 3H), 7.24 – 7.20 (m, 2H), 7.15 – 7.04 (m, 3H), 5.44 (dd, *J* = 5.8, 2.6 Hz, 1H), 3.69 (dd, *J* = 13.2, 2.7 Hz, 1H), 3.65 – 3.56 (m, 2H), 3.35 (dd, *J* = 14.3, 7.3 Hz, 1H), 1.33 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.62 , 143.61 , 132.84 , 132.15 , 128.67 , 128.31 , 128.16 , 128.07 , 126.39 , 123.84 , 122.29 , 59.34 , 47.92 , 31.48 , 6.38 . HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₇H₁₈NO₃SSe 396.0167 found 396.0169.



3-((phenylselanyl)methyl)isobenzofuran-1(3H)-one **(5)**. Colorless oil (88%, 0.133g). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 7.4 Hz, 1H), 7.42 (td, *J* = 7.4, 1.3 Hz, 1H), 7.39 – 7.33 (m, 2H), 7.33 – 7.28 (m, 2H), 7.13 – 7.04 (m, 3H), 5.51 (t, *J* = 5.5 Hz, 1H), 3.30 (dd, *J* = 13.3, 5.1 Hz, 1H), 3.22 (dd, *J* = 13.3, 5.9 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 170.02, 148.54, 133.99, 133.53, 129.53, 129.26, 129.21, 127.69, 126.50, 125.50, 122.54, 79.15, 31.92. HRMS (TOF) m/z [M + H]⁺ Calcd for C₁₅H₁₃O₂Se 305.0075 found 305.0080.

11. ¹H NMR, ¹³C NMR and ¹⁹F NMR spectra













HJW-20200108-3.7.1.1r





20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 f1 (ppm)



















Product 3k






20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 f1 (ppm)









210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)













































Product 3ai













210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

Product 4b





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

Product 4d





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

-0.00





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)









210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)



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